Molecular Dynamics Simulation of Nucleation of SWNT from a Metal Particle on a Substrate

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Nucleation process of single-walled carbon nanotubes (SWNTs) from a transition metal cluster on a substrate is studied using classical molecular dynamics (MD) simulations. In our previous study, nucleation process of SWNTs from a non-supported catalytic metal cluster such as floated CVD process was performed using classical MD methods [1]. Recently, vertically aligned high-quality SWNTs on quartz substrates have been produced using the Alcohol CCVD method [2]. Here, initial nucleation process of SWNTs from the catalytic metal cluster on a substrate is calculated using classical MD methods.

Simulation technique is the same as our previous work [1] expect for a few points. Mirror boundary is used for top and bottom boundary. For describing the effect of the substrate, averaged one-dimensional Lennard-Jones potential is employed between the metal cluster and the bottom boundary of the simulation cell. As the initial condition, a Ni_{500} cluster is placed on the bottom boundary of the cubic cell of 20 nm. The number of carbon atoms is adjusted to achieve the constant density by adding a new carbon atom to the cell when the metal cluster dissolves a carbon atom. Figure 1 shows snapshots of initial nucleation process of carbon atoms from a metal cluster on a substrate. As the metal cluster dissolves carbon atoms, the cluster becomes more wetting to the substrate. This may be due to the different wettability between pure metal and metal-carbide. Graphite structure gradually precipitates from the edge of the cluster. Nucleation mechanism of SWNTs will be discussed with continued simulation results, which may reach to the nucleation of a cap structure of an SWNT.

[1] Y. Shibuta, S. Maruyama, Chem. Phys. Lett., 382 (2003) 381. [2] Y. Murakami, S. Chiashi, Y. Miyauchi, M. Hu, M. Ogura, T. Okubo, S. Maruyama, Chem. Phys. Lett., 385 (2004) 298.

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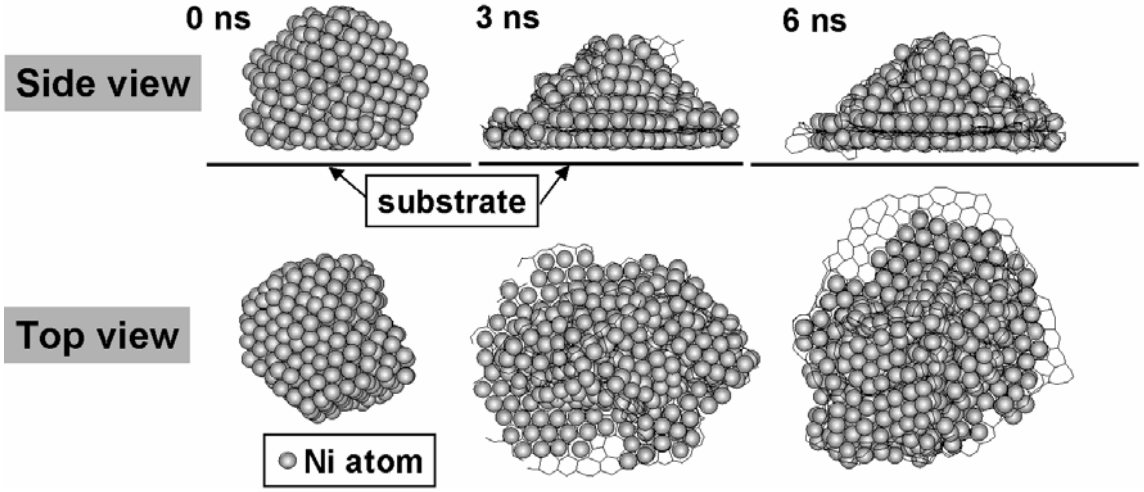

Fig. 1 Snapshots of initial nucleation process of graphitic carbon atoms from Ni_{500} cluster on a substrate.